7 pages

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ON THE USE OF THIELE'S SEMI-INVARIANTS IN FERROMAGNETISM*

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by

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In the spinwave model of ferromagnetism, the physical restriction that not more than 2S units of reversed spin can come together on the same atom leads to what Dyson [1] has called the kinematical interaction. This letter indicates a method of calculating the effect of these interactions on the temperature dependence of the magnetization by using the semi-invariants of Thiele [2].

The nearest neighbor exchange interaction model is described by the Hamiltonian

$$\mathcal{H} = -2J \sum_{<ij>} \underset{\sim}{S}_i \cdot \underset{\sim}{S}_j + g\mu H \sum_{i=1}^{N} S_i^{z} \tag{1}$$

$\underset{\sim}{S}$ is the spin operator at the i-th atom, g the Landeʹ g-factor, H the magnetic field in the z direction, $\mu = eh/mc$, $\sum_{<ij>}$ is taken over all nearest neighbor pairs, and N is the number of atoms.

Following Holstein and Primakoff [3] and Oguchi [4], the spin operators are replaced by the spin deviation creation and annihilation operators $a^\dagger$ and a. At low temperatures, where the number of spin deviations is expected to be very small, the Hamiltonian may be linearized to

$$\mathcal{H} = -[JzNS^2 - g\mu HNS] - 2JS \sum_{<ij>} [a_i^\dagger a_j + a_i a_j^\dagger]$$
$$-2JS \sum_{<ij>} [a_i^\dagger a_i + a_j^\dagger a_j] - g\mu H \sum_i a_i^\dagger a_i \tag{2}$$

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where z is the number of nearest neighbors.

By introducing the spinwave operators $b_{\mathbf{k}} = (1/N^{\frac{1}{2}}) \sum_j \exp(i\mathbf{k}\cdot\mathbf{R}_j)\, a_j$ and $b_{\mathbf{k}}^\dagger = (1/N^{\frac{1}{2}}) \sum_j \exp(-i\mathbf{k}\cdot\mathbf{R}_j)\, a_j^\dagger$, the Hamiltonian is Fourier transformed to

$$\mathcal{H} = \mathcal{H}_o + \Sigma_{\mathbf{k}} A_{\mathbf{k}} n_{\mathbf{k}} \tag{3}$$

Here $\mathcal{H}_o = -[JzNs^2 - g\mu HNS]$, $A_{\mathbf{k}} = [2JSz(1-\gamma_{\mathbf{k}}) - g\mu H]$, $n_{\mathbf{k}} = b_{\mathbf{k}}^\dagger b_{\mathbf{k}}$, $\gamma_{\mathbf{k}} = (1/z) \sum_\rho \exp(i\mathbf{k}\cdot\mathbf{R}_\rho)$ and ρ is the vector between nearest neighbor atoms.

In equation (3), $\mathcal{H}_o$ is the Hamiltonian of the free spin-waves, and $\sum_{\mathbf{k}} A_{\mathbf{k}} n_{\mathbf{k}}$ represents the interactions. The partition function of the system is then defined by

$$\begin{aligned} Z &= \text{Trace} \exp(-\beta\mathcal{H}), \quad \beta = 1/kT \\ &= \exp(-\beta\mathcal{H}_o) \text{ trace} \exp(-\beta\textstyle\sum_{\mathbf{k}} A_{\mathbf{k}} n_{\mathbf{k}}) \\ &= Z_o Z_1 \end{aligned} \tag{4}$$

We will now evaluate $Z_1 = \text{trace} \exp(-\beta\sum_{\mathbf{k}} A_{\mathbf{k}} n_{\mathbf{k}})$ for two cases. In the ideal case the assumption is made that the only effect of the kinematical interaction is to restrict the maximum permissible eigenvalue of the spinwave operator $n_{\mathbf{k}}$ to 2S, and that the interactions of the spinwaves with each other may be neglected. This is mathematically equivalent to neglecting the cross terms in $(\sum_{\mathbf{k}} A_{\mathbf{k}} n_{\mathbf{k}})^r$. Thus

$$\begin{aligned} Z_1 &= \sum_{n_{\mathbf{k}}=0}^{2S} \exp(-\beta \textstyle\sum_{\mathbf{k}} A_{\mathbf{k}} n_{\mathbf{k}}) \\ &= \prod_{\mathbf{k}} \left[\left\{1-\exp[-(2S+1)\beta A_{\mathbf{k}}]\right\} / \left\{1-\exp(-\beta A_{\mathbf{k}})\right\} \right] \end{aligned} \tag{5}$$

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and $$\ln Z_1 = \sum_{k} \ln\left[\left\{1-\exp[-(2S+1)\beta A_k]\right\} / \left\{1-\exp(-\beta A_k)\right\}\right] \tag{6}$$

Alternately

$$\ln Z_1 = \ln \text{ trace } \exp\left(-\beta \sum_k A_k n_k\right)$$
$$= \ln \text{ trace } (1) + \ln\left[1 + \sum_{r=1} \frac{(-\beta)^r}{r!} M(r)\right] \tag{7}$$

where the r-th moment of the Hamiltonian, $M(r) = \text{trace } (\sum_k A_k n_k)^r /$ trace (1), has been set equal to trace $(\sum_k A_k^r n_k^r)$/trace (1), and trace$(1) = (2S+1)^N$.

When the second term in equation (7) is expanded,

$$\ln Z_1 = \ln (2S+1)^N + \sum_{m=1} \frac{(-\beta)^m}{m!} \lambda(m) \tag{8}$$

Here $\lambda(m)$, the m-th semi-invariant of Thiele, is the sum of the coefficients of β^m in the expansion. The first three semi-invariants are [5],

$$\lambda(1) = M(1) \tag{9}$$

$$\lambda(2) = M(2) - M^2(1) \tag{10}$$

$$\lambda(3) = M(3) - 3M(2)M(1) + 2M^3(1) \tag{11}$$

However, from equation (6) it is not difficult to show that

$$\lambda(m) = \frac{(-)^m}{m} B_m \left[(2S+1)^m - 1\right] \sum_k A_k^m \tag{12}$$

where B_m are the well known Bernoulli numbers. Thus

$$\lambda(1) = S \sum_k A_k \tag{13}$$

$$\lambda(2) = \frac{1}{3} S(S+1) \sum_k A_k^2 \tag{14}$$

$$\lambda(3) = 0 \cdot \sum_k A_k^3 \tag{15}$$

Equation (8) may then be replaced by

$$\ln Z_1 = \ln (2S+1)^N - S\beta \sum_{\underline{k}} A_{\underline{k}} + \tfrac{1}{3} S(S+1)\beta^2 \sum_{\underline{k}} A_{\underline{k}}^2 - 0 + \cdots \quad (16)$$

In tho cxact caso, whoro the intoraction of the spinwaves with each other is specifically accounted for, it becomes necessary to evaluate the cross terms arising in trace$(\sum A_{\underline{k}} n_{\underline{k}})^n$. Methods of doing this will be presented elsewhere. It is found that the first three semi-invariants are

$$\lambda(1) = S \sum_{\underline{k}} A_{\underline{k}} \quad (17)$$

$$\lambda(2) = S^2 \sum_{\underline{k}} A_{\underline{k}}^2 - \tfrac{1}{3} S(2S+1) \frac{1}{N} \sum_{\underline{k}_1} \sum_{\underline{k}_2} A_{\underline{k}_1}^2 A_{\underline{k}_2} \quad (18)$$

$$\begin{aligned}\lambda(3) &= 2S^3 \sum_{\underline{k}} A_{\underline{k}}^3 - S^2 (4S+1) \frac{1}{N} \sum_{\underline{k}_1} \sum_{\underline{k}_2} A_{\underline{k}_1}^2 A_{\underline{k}_2} \\ &\quad + S^2 (2S+1) \frac{1}{N^2} \sum_{\underline{k}_1} \sum_{\underline{k}_2} \sum_{\underline{k}_3} A_{\underline{k}_1} A_{\underline{k}_2} A_{\underline{k}_3}\end{aligned} \quad (19)$$

The effect of the interacting spinwaves is to introduce higher order sums in k-space and to alter the coefficients of the first order summation. The details of this calculation show a resemblance to the classical rencontre problem in the theory of games [5], and from this a conjecture is made that the coefficient of $(\sum_{\underline{k}} A_{\underline{k}}^m)$ is $(m-1)!\, S^m$. Thus

$$\lambda(m) = (m-1)! \sum_{\underline{k}} (S A_{\underline{k}})^m \quad (20)$$

and

$$\ln Z_1 = \ln (2S+1)^N + \sum_{m>1} \sum_{\underline{k}} (-S\beta A_{\underline{k}})^m \quad (21)$$

$$= \ln (2S+1)^N + \sum_{\underline{k}} \ln (1 + S\beta A_{\underline{k}}) \quad (22)$$

The magnetization is calculated in the standard manner. For the ideal (non-interacting) case

(23)

$$\frac{M(\beta)}{M(\infty)} = 1 - \frac{1}{S}\sum_{m=1} \Big[(2S+1)\exp[-12m(2S+1)x]\, I_0^3[4m(2S+1)x] - \exp(-12mx)\, I_0^3(4mx)\Big] \quad \ldots\ldots \tag{23}$$

where $x=\beta JS$ and we have set $z=6$.

At very low temperatures an asymptotic expansion gives

$$\frac{M(\Theta)}{M(0)} = 1 - \frac{1}{S}\Big[f_{3/2}(S)a_0\,\Theta^{3/2} + f_{5/2}(S)a_1\,\Theta^{5/2} + f_{7/2}(S)a_2\,\Theta^{7/2} + \cdots\Big] \tag{24}$$

where $\Theta = kT/6\pi JS$ and $f_{n/2}(S) = 1 - (1+2S)^{-n/2}$

The coefficients a_0, a_1, a_2 are identical to Dyson's. This method does not give integer powers of the temperature probably becuase the interaction of the spinwaves with each other was neglected. But it is interesting to note that the modifying factor $f_{n/2}(S)$ becomes unity in the limit of $S \to \infty$

In the exact (interacting) case, the magnetization has been obtained in integral form

$$\frac{M(\Theta)}{M(0)} = 1 - \frac{1}{S}\,2\pi\Theta\,\frac{1}{(2\pi)^3}\int_0^{2\pi}\!\!\int_0^{2\pi}\!\!\int_0^{2\pi}\frac{d\varphi_1\, d\varphi_2\, d\varphi_3}{(3+2\pi\Theta/S) - (\cos\varphi_1 + \cos\varphi_2 + \cos\varphi_3)} \tag{25}$$

The second term is a direct consequence of the conjecture made earlier which is rendered plausible by the similarity to the generalized Watson's integral which has an interesting history in the spinwave theory of ferromagnetism[6].

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